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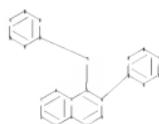
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chain nodes :
23
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22
chain bonds :
7-23 8-12 22-23
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 11-12 11-16 12-13 13-14
14-15 15-16 17-18 17-22 18-19 19-20 20-21 21-22
exact/norm bonds :
7-23 22-23
exact bonds :
8-12
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 11-12 11-16 12-13 13-14
14-15 15-16 17-18 17-22 18-19 19-20 20-21 21-22
isolated ring systems :
containing 1 : 11 : 17 :

G1:O,S

Match level :

04/17/2008

10-598,246.trn

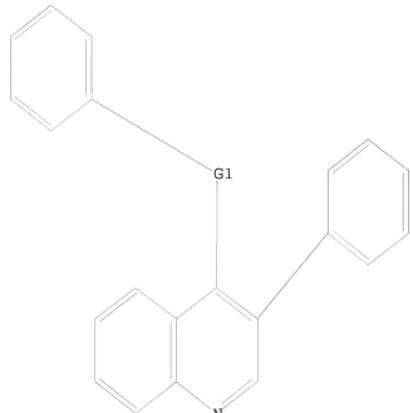
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 22:Atom 23:CLASS

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR



G1 O,S

Structure attributes must be viewed using STN Express query preparation.

=> s 11 sss sam

SAMPLE SEARCH INITIATED 12:55:24 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 9 TO ITERATE

100.0% PROCESSED 9 ITERATIONS
SEARCH TIME: 00.00.01

1 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 9 TO 360
PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

04/17/2008

10-598,246.trn

=> s 11 sss full
FULL SEARCH INITIATED 12:55:33 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 122 TO ITERATE

100.0% PROCESSED 122 ITERATIONS 25 ANSWERS
SEARCH TIME: 00.00.01

L3 25 SEA SSS FUL L1

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COST IN U.S. DOLLARS SINCE FILE TOTAL
FULL ESTIMATED COST ENTRY SESSION 179.49
179.28

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=> s 13
L4 5 L3

=> d ibib abs hitstr 1-
YOU HAVE REQUESTED DATA FROM 5 ANSWERS - CONTINUE? Y/(N):y

14 NUMBER 3 OF 3 CAPTION COPYRIGHT 2020 ACS OF STN (Continued)

333 02030-11-6 CAPLUS
CN 2-Propenoic acid,
3-[4-[(2-ethyl-7-hydroxy-3-[3-(trifluoromethyl)phenyl]-4-
quinoxaling-1-oxo)phenyl]- (CA INDEX NAME)

INN 820300-14-7 CAPLUS
CII 2-Propenoic acid, 3-[3-[(2-ethyl-7-hydroxy-3-phenyl-4-methylsulfonyl)oxy]phenyl]- [CA INDEX NAME]

14 APPENDIX 3 OF 5 CARDS COPYRIGHT 2008 ACS on 8/28 (Continued)

INN 863711-18-6 CAPLUS
 CN 2-Propanamide,
 3-[4-[(2-ethyl-7-hydroxy-3-phenyl-4-quinoliny1)thio]phenyl]-
 1,1-DIHYDRO-NAPHTHA[1,2-C]THIOPHENE

IT 883713-19-7
Ms. RCT (Reagent); RACT (Reagent or reagent)
(Preparation of substituted quinoline compounds for use as selective
antiprotozoal agents to treat various diseases)
IN 883713-19-7
CN 2-(4-chlorophenyl)-4-(4-chlorophenyl)-1,2-dihydro-1,4-dihydroquinoline-1,4-dione
CA INDEX NAME

CN 7-Quinolinol, 4-(4-bromophenoxy)-2-ethyl-3-phenyl- (CA 18(9): 8946)

14 ANNEX 1 OR 5 CARBON COPYRIGHT 2008 ACE OR ETHE (Continued)

RE 063711-16-4 CAPROS
CN 2-Propenenitrile, 3-[4-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyloxy)oxy]phenyl]- (CA INDEX NAME)

RR 063711-17-5 CAP108
CN 2-Propenamide, 3-[4-[(2-ethyl-7-hydroxy-3-[3-(trifluoromethyl)phenyl]-4-quinolinyl)oxy]phenyl]-N-(1-methylethyl)- (CA INDEX RRN8)

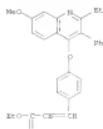
14 ANSWER 3 OF 5 CAPTION COPYRIGHT 2008 ACS on STN (Continued)

IT 82300-18-1, 2-Ethyl-3-phenyl-4-(4-bromophenoxy)-7-methoxyquinoline 82300-18-1
 KLT NCT (Reactant); RIM (Synthetic preparation); PREP (Preparation); NACT (Reactant or reagent)
 (preparation of substituted quinoline compds. for use as selective estrogen receptor modulator to treat various diseases)
 RM 82300-18-1 CAPIUS
 CA Quinoline, 4-(4-bromophenoxy)-2-ethyl-7-methoxy-3-phenyl- (CA INDEX

The chemical structure shows a chromene core (a benzene ring fused to a five-membered ring) with a methoxy group (-MeO) at position 2 and a phenyl group at position 7. The five-membered ring has a double bond between the 4 and 5 positions.

INN 828200-22-7 CAPLUS
CN 2-Propenoic acid, 3-[4-[(2-ethyl-7-methoxy-3-phenyl)-4-

14 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

14 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

2004-107397 CAPLUS
ACCesion NUMBER: 142123080
DOCUMENT NUMBER:
TITLE: Discovery of Novel Quinoline-Based Estrogen Receptor Ligands Using Peptide Interaction Profiling
Hockstra, William J.; Patel, Mai S.; Liang, Xj; Hwang, Daniel; Lai, Ming; Li, Ming; Liu, Yiqun; Tinsley, M.; Iannone, Marie A.; Kuchell, Sue M.; Miller, Lisa A.; Pearce, Kenneth H.; Summons, Robert; GlaxoSmithKline Research Development, Research Triangle Park, NC 27709-3799, USA
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142123080
AS Traditional approaches to discover new estrogen receptor modulators (ERMs) have relied on cell binding and cell-based estrogen response element-driven assays to identify compounds that are estrogenic but nonproliferative in breast and uterine tissues. To discover novel ERM candidates, we have developed an ERM-free microspheres-based binding assay to rapidly characterize ERM interactions with conformation-sensing conforstar or phage display peptides. Peptide profiles of constrained triketones were compared to known estrogen receptor ligands to identify novel ERM candidates. We discovered potent quinoline-based ligands with minimal late-stage cell stimulation. 17 828390-07-89 828390-09-99 828390-09-09 828390-10-09 828390-11-10 828390-12-11 828390-13-12 828390-14-79 828390-15-89 828390-16-90 828390-17-91 828390-18-92 828390-19-93 828390-20-94 828390-21-95 828390-22-96 828390-23-97 828390-24-98 828390-25-99 828390-26-00 828390-27-01 828390-28-02 828390-29-03 828390-30-04 828390-31-05 828390-32-06 828390-33-07 828390-34-08 828390-35-09 828390-36-10 828390-37-11 828390-38-12 828390-39-13 828390-40-14 828390-41-15 828390-42-16 828390-43-17 828390-44-18 828390-45-19 828390-46-20 828390-47-21 828390-48-22 828390-49-23 828390-50-24 828390-51-25 828390-52-26 828390-53-27 828390-54-28 828390-55-29 828390-56-30 828390-57-31 828390-58-32 828390-59-33 828390-60-34 828390-61-35 828390-62-36 828390-63-37 828390-64-38 828390-65-39 828390-66-40 828390-67-41 828390-68-42 828390-69-43 828390-70-44 828390-71-45 828390-72-46 828390-73-47 828390-74-48 828390-75-49 828390-76-50 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828390-742-716 828390-743-717 828390-744-718 828390-745-719 828390-746-720 828390-747-721 828390-748-722 828390-749-723 828390-750-724 828390-751-725 828390-752-726 828390-753-727 828390-754-728 828390-755-729 828390-756-730 828390-757-731 828390-758-732 828390-759-733 828390-760-734 828390-761-735 828390-762-736 828390-763-737 828390-764-738 828390-765-739 828390-766-740 828390-767-741 828390-768-742 828390-769-743 828390-770-744 828390-771-745 828390-772-746 828390-773-747 828390-774-748 828390-775-749 828390-776-750 828390-777-751 828390-778-752 828390-779-753 828390-780-754 828390-781-755 828390-782-756 828390-783-757 828390-784-758 828390-785-759 828390-786-760 828390-787-761 828390-788-762 828390-789-763 828390-790-764 828390-791-765 828390-792-766 828390-793-767 828390-794-768 828390-795-769 828390-796-770 828390-797-771 828390-798-772 828390-799-77

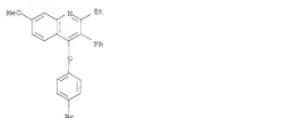
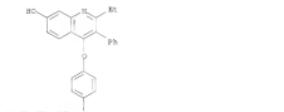
14 ARIZMENDI, 2 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

322 626300-12-5 CAPLUS
C2 2-Propenoic acid,
3-[4-(17-hydroxy-2,3-diphenyl-4-quinolinyl)oxy]phenyl 1-
ICA INDEX NAME



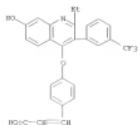
INN 828300-13-6 CAPROS
CN 2-Propenoic acid,
3-[4-((2-ethyl-7-hydroxy-3-[(3-(trifluoromethyl)phenyl)-4-
quinoxalinyl]oxy)phenyl)- (CA INDEX NAME)

14 ANSWER 2 OF 5 CAPTION COPYRIGHT 2008 ACS on 979 (Continued)

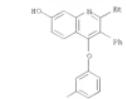


INN 829300-19-2 CAPTUS
CN Quinoline, 4-(4-bromophenoxy)-7-methoxy-2,3-diphenyl- (CA INDEX NAME)

L6 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2008 ACS on 5TH (Continued)

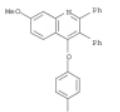


INN: 828300-14-7 CAPLOS
CN: 2-Propenoic acid, 3-[3-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyloxy)phenyl]- (CA INDEX NAME)

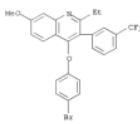


RI 828300-15-8 CAPI08
CS 7-Quinolinol, 4-[4-(2-(dimethylamino)ethoxy)phenoxy]-2-ethyl-3-phenyl
(CA INDEX NAME)

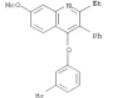
1.6 ANSWER 2 OF 5 CAPTION COPYRIGHT 2008 ACS on 87N (Continued)



INN 828300-20-5 CAP105
CII Quinoline, 4-(4-bromophenoxy)-2-ethyl-7-methoxy-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RR 828300-21-6 CAPIUS
CN Quinoline, 4-(3-bromophenoxy)-2-ethyl-7-methoxy-3-phenyl- (CA INDEX NAME)



BN 828300-22-7 CAPLUS
CN 2-Propenoic acid, 3-[4-[(2-ethyl-7-methoxy-3-phenyl-4-quinolinyloxy)phenyl]-, ethyl ester (CA INDEX NAME)

14 ANGELICA 5 OR 6 CAPSULES. COPPER(II) 3239 ACT on 27H [Continued]
mol. PdH2 give 539 V, 0.07 mol. 1 and 0.04 mol. PdH2 give 55 V, 228 IV,
and 1.7 g. [PdH2] 200. The PdH2C1C9H20C2H2O2 (from 3.8 g. 1 and 1.7 g.
PdH2) gives 539 V, 0.07 mol. PdH2, gives 47 and 514 V, resp.
15 600719-93-2, 4-Phenyl-6-phenyl-4-phenoxyl-3-phenyl-
Ela FPEP (Preparation)
16 600719-93-2, CAPTUS
Quinoline, 4-phenyl-4-phenoxyl-3-phenyl- (CA INDEX NAME)



04/17/2008

10-598,246,trn

二〇

---Logging off of STN---

2

Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	43.57	223.06
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)		SINCE FILE
		ENTRY
CA SUBSCRIBER PRICE	-4.00	-4.00

STN INTERNATIONAL LOGOFF AT 13:16:01 ON 15 APR 2008

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID: septaijem1625

PASSWORDS

PASSWORD: TERMINAL (ENTER 1, 2, 3, OR ?):?

NEWS 13 FEB 29 WPINDEX/WPIDS/WPIX enhanced with ECLA and current U.S. National Patent Classification
NEWS 14 MAR 31 IFICDB, IFIPAT, and IFIUDB enhanced with new custom IPC display formats
NEWS 15 MAR 31 CAS REGISTRY enhanced with additional experimental spectra
NEWS 16 MAR 31 CA/Caplus and CASREACT patent number format for U.S. applications updated
NEWS 17 MAR 31 LPCI now available as a replacement to LDPCI
NEWS 18 MAR 31 EMBASE, EMBAL, and LEMBASE reloaded with enhancements
NEWS 19 APR 04 STA AnaVist, Version 1, to be discontinued
NEWS 20 APR 15 WPIDS, WPINDEX, and WPIX enhanced with new predefined bit display formats

NEWS EXPRESS FEBRUARY 08 CURRENT WINDOWS VERSION IS V8.3,
AND CURRENT DISCOVER FILE IS DATED 20 FEBRUARY 2008

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items
NEWS IPC8 For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

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=> FIL REGISTRY
COST IN U.S. DOLLARS
SINCE FILE
ENTRY
SESSION
TOTAL
0.21
0.21

FILE 'REGISTRY' ENTERED AT 14:51:43 ON 16 APR 2008
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STRUCTURE FILE UPDATES: 15 APR 2008 HIGHEST RN 1015083-77-8

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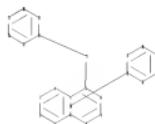
TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>
Uploading C:\Program Files\Stnexp\Queries\10-598,246a.str



```
chain nodes :  
23  
ring nodes :  
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22  
chain bonds :  
7-23 22-23  
ring bonds :  
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 11-12 11-16 12-13 13-14  
14-15 15-16 17-18 17-22 18-19 19-20 20-21 21-22
```

04/17/2008

10-598,246.trn

exact/norm bonds :

7-23 22-23

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 11-12 11-16 12-13 13-14
14-15 15-16 17-18 17-22 18-19 19-20 20-21 21-22

isolated ring systems :

containing 1 : 11 : 17 :

G1:O,S

Match level :

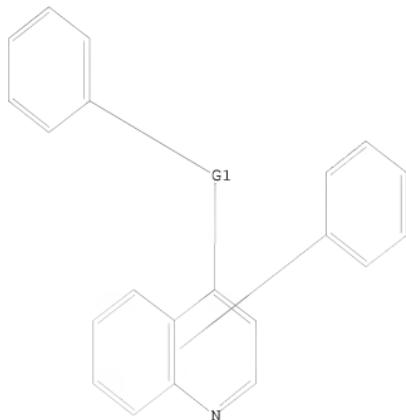
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 22:Atom 23:CLASS 26:Atom

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR



G1 O,S

Structure attributes must be viewed using STN Express query preparation.

```
=> s 11 sss sam
SAMPLE SEARCH INITIATED 14:52:24 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      469 TO ITERATE

100.0% PROCESSED      469 ITERATIONS          3 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:      8081 TO      10679
PROJECTED ANSWERS:          3 TO       163

L2      3 SEA SSS SAM L1

=> s 11 sss full
FULL SEARCH INITIATED 14:52:36 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      9410 TO ITERATE

100.0% PROCESSED      9410 ITERATIONS          105 ANSWERS
SEARCH TIME: 00.00.01

L3      105 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS          SINCE FILE      TOTAL
                                ENTRY      SESSION
FULL ESTIMATED COST          178.82      179.03

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<http://www.cas.org/infopolicy.html>

=> s 13

04/17/2008

10-598,246.trn

L4 25 L3

=> d ibib abs hitstr l-
YOU HAVE REQUESTED DATA FROM 25 ANSWERS - CONTINUE? Y/(N):y

LA ANSWER 1 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 148113983125 CAPLUS

DOCUMENT NUMBER: 148113983204 CAPLUS

TITLE: A series of protease inhibitors by modifying of helicase residues in hepatitis C virus nonstructural protein 3

AUTHOR(S): Nekhlyudov, Svetlana; Gerasimov, Anna; Askarov, Eva; Hanekom, U. Helma

CORPORATE SOURCE(S): Department of Biochemistry and Organic Chemistry, University of Utrecht, The Netherlands

SOURCE(S): EURE Journal (2007), 27(42), 5979-5986

PUBLISHER: Elsevier Publishing Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

ABSTRACT: This study of the full-length multifunctional nonstructural protein 3 from hepatitis C virus (HCV) has revealed that residues in the helicase domain of the protein, which are involved in the interaction with the 5' untranslated region, apparently located in the interface between the 3D and 5D binding pockets of the substrate binding site of the protease, were selected for modification. A series of 10 substituted nonstructural protein 3s were expressed, purified and characterized. The substitutions resulted in indistinguishable Km values and slightly lower *Ki* values compared to the wild-type. The *Ki* values for a series of structurally diverse protease inhibitors were affected by the substitutions, with increases or decreases up to 10-fold. The inhibition profiles for H328A and H328S were similar, but the H328T substitution, which did not change the side chain, had an effect, but also that minor differences in the nature of the introduced side chain influenced the characteristics of the enzyme.

These results indicate that residues in the helicase domain of nonstructural protein 3 can influence the protease, supporting our hypothesis that full-length hepatitis C virus nonstructural protein 3 should be used for the design of potent and selective protease inhibitors. The data suggest that inhibitors can be designed to interact with residues in the helicase domain potentially leading to more potent and selective

1021131-39-0

ELI AUZ [Analytical role, unclassified]; EUD [Biological study, unclassified]; EUN [Analytical study]; EUD [Biological study]; [inhibitor H3 protease activity; identification of residues in helicase domain of HCV protein H3 that affect inhibition of protease activity]

1021131-39-0 CAPLUS

CHS [[(2R)-2-((1R)-2-((1R)-2-((1R)-2-((1R)-2-((1R)-2-

[(1R)-2-((1R)-2-((1R)-2-((1R)-2-((1R)-2-((1R)-2-((1R)-2-

,1,1-dianethyllethyl)ester (CA INDEX NAME)]

Absolute stereochemistry.

LA ANSWER 2 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005124155 CAPLUS

DOCUMENT NUMBER: 148113983205 CAPLUS

TITLE: Phenylglycine as a novel P2 scaffold in hepatitis C virus H3 protease inhibitors

AUTHOR(S): Gerasimov, Anna; Nekhlyudov, Svetlana; Askarov, Eva; Gossas, Thomas; Sabina, Yeganeh A.; Fransson, Magnus; Lindberg, Gunnar; Hanekom, U. Helma; Nekhlyudov, Svetlana; Gerasimov, Anna

CORPORATE SOURCE(S): Department of Medicinal Chemistry, RMC, Uppsala University, Uppsala, SE-751 23 Uppsala, Sweden; Department of Organic Chemistry (2007), 35(3), 1446-1474

PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 146:287649

ABSTRACT: New modeling and inhibitory potencies of tetrapeptide protease inhibitors

models based on HCV H3 proposed phenylglycine as a new proline P2 residue. The phenylglycine residue was found to be a good P2 residue in combination with the H31 (protease-helicase/NTFase) in ways not possible for the common P2 proline-based inhibitors. Thus, a series of tripeptides, both linear and cyclic, were synthesized and their inhibitory effect determined. When the p-hydroxy group was

replaced by methoxy, isopropylidene-, or guanidinoxy functions, inhibitors with improved potencies were obtained. The P2 phenylglycine-based inhibitors were further optimized by C-terminal extension to acyl tetrapeptides and the resulting compounds gave products with

inhibition in the nanomolar range (approx. 70 nM).

1021132-22-25 928162-49 928162-57-45

ELI DNA [Drug mechanism of action]; EUD [Pharmacological activity]; ECT [Experimental use]; EUD [Biological study]; PRED [Preparation]; RCT [Reagent or reagent]; USES [Uses]; USES [Uses]

H3 protease: Hepatitis C virus H3 protease inhibitors preparation: phenylglycine

as novel P2 scaffold

1021132-22-25 CAPLUS

CHS Cyclopropanearboxylic acid,

N-[1,1,1,1-dianethyllethoxy]oxybenzoyle-2-L-valyl-1-(2S-

-2-[4-((1-methoxy-2-phenyl-4-quinolinyloxy)phenyl)glycyl-L-amino-2-ethenyl-
(2S,2R)-] (CA INDEX NAME)

Absolute stereochemistry.

LA ANSWER 1 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

148113983125 CAPLUS

148113983204 CAPLUS



REFERENCE COUNT: THIS

30 THREE ARE 20 CITED REFERENCES AVAILABLE FOR RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

FORMAT

LA ANSWER 2 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

2005124155 CAPLUS

148113983205 CAPLUS

TITLE: Phenylglycine as a novel P2 scaffold in hepatitis C virus H3 protease inhibitors

AUTHOR(S): Gerasimov, Anna; Nekhlyudov, Svetlana; Askarov, Eva; Gossas, Thomas; Sabina, Yeganeh A.; Fransson, Magnus; Lindberg, Gunnar; Hanekom, U. Helma; Nekhlyudov, Svetlana; Gerasimov, Anna

CORPORATE SOURCE(S): Department of Medicinal Chemistry, RMC, Uppsala University, Uppsala, SE-751 23 Uppsala, Sweden; Department of Organic Chemistry (2007), 35(3), 1446-1474

PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 146:287649

ABSTRACT: New modeling and inhibitory potencies of tetrapeptide protease

inhibitors

models based on HCV H3 proposed phenylglycine as a new proline P2 residue.

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the H31 (protease-helicase/NTFase) in ways not possible for the common P2 proline-based inhibitors. Thus, a series of tripeptides, both linear and cyclic, were synthesized and their inhibitory effect determined. When the p-hydroxy group was

replaced by methoxy, isopropylidene-, or guanidinoxy functions, inhibitors with

improved potencies were obtained. The P2 phenylglycine-based

inhibitors were further optimized by C-terminal extension to acyl

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1021132-22-25 928162-49 928162-57-45

ELI DNA [Drug mechanism of action]; EUD [Pharmacological activity]; ECT [Experimental use]; EUD [Biological study]; PRED [Preparation]; RCT [Reagent or reagent]; USES [Uses]; USES [Uses]

H3 protease: Hepatitis C virus H3 protease inhibitors preparation: phenylglycine

as novel P2 scaffold

1021132-22-25 CAPLUS

CHS Cyclopropanearboxylic acid,

N-[1,1,1,1-dianethyllethoxy]oxybenzoyle-2-L-valyl-1-(2S-

-2-[4-((1-methoxy-2-phenyl-4-quinolinyloxy)phenyl)glycyl-L-amino-2-ethenyl-
(2S,2R)-] (CA INDEX NAME)

Absolute stereochemistry.

CHS 928162-23-6 CAPLUS

CH Butanoic acid,

N-[1,1-dimethyllethoxy]carbonyl-3-methyl-1-*l*-valyl-1-(2S)-2-[4-((1-methoxy-2-phenyl-4-quinolinyloxy)phenyl)glycyl-2-amino-4,4-difluoro-
(2S)-] (CA INDEX NAME)

Absolute stereochemistry.

CHS 928162-23-6 CAPLUS

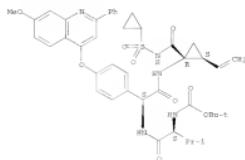
CH Butanoic acid,

N-[1,1-dimethyllethoxy]carbonyl-3-methyl-1-*l*-valyl-1-(2S)-2-[4-((1-methoxy-2-phenyl-4-quinolinyloxy)phenyl)glycyl-2-amino-4,4-difluoro-
(2S,2R)-] (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

14 ANSWER 2 OF 25 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)



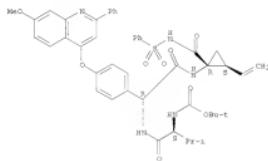
15 928162-62-3 CAPLUS
 CH₃ Citramalic acid, N-(11b,45,79,128,155)-4-[4-[(7-methoxy-2-phenyl-4-quinolinyl)oxy]phenyl]-3,6-dioxo-1-[(phenylsulfonyl)amino]carbonyl-2,5-dioxo-1,2,3,4-tetrahydro-1,1,2,3,4,5-hexadec-13-en-7-yl-, 1,1-dimethylethyl ester (CA INDEX NAME)

Absolute stereochemistry:
 Double bond geometry as shown.



16 928162-61-2 CAPLUS
 CH₃ Citramalic acid,
 N-[(11b,45,79,128,158)-1-[(cyclopropylsulfonyl)amino]carbo-

14 ANSWER 2 OF 25 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)



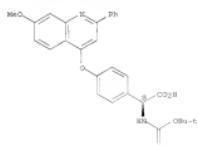
17 928162-13-4P 928162-18-9P 928162-19-3P
 928162-20-3P 928162-21-4P 928162-25-8P
 928162-26-9P 928162-27-0P 928162-28-1P
 928162-29-2P 928162-31-5P 928162-54-3P
 945904-19-7P 945904-35-8P 945904-91-0P
 945904-92-1P 945904-93-2P 945904-94-3P
 KL NCT (Meatant); 9MP (Synthetic preparation); PMP (Preparation); RACT (Meatant); RACT (Synthetic preparation); NH3 protease inhibitors preparation: phenylglycine

44 novel PI scaffold

928162-13-4 CAPLUS

CH₃ Phenazeneacetic acid, 4-[(1,1-dimethylhexyl)amino]-4-[(7-methoxy-2-phenyl-4-quinolinyl)oxy]-, (2S)- (CA INDEX NAME)

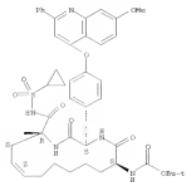
Absolute stereochemistry.



18 928162-18-9 CAPLUS
 CH₃ Cyclopropanecarboxylic acid, 2-[(12b)-3,6-dioxo-1-

14 ANSWER 2 OF 25 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)
 yl-4-[(17-methoxy-2-phenyl-4-quinolinyl)oxy]phenyl]-3,6-dioxo-2,5-diaza-3-cyclo[13.3.0]hexadec-13-en-7-yl-, 1,1-dimethylethyl ester (CA INDEX NAME)

Absolute stereochemistry:
 Double bond geometry as shown.

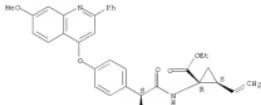


15 928162-18-7 CAPLUS
 CH₃ Cyclopropanecarboxamide, N-[(1,1-dimethylhexyl)carbonyl]-L-valyl-(2S)-4-[(17-methoxy-2-phenyl-4-quinolinyl)oxy]phenyl-1-glycyl-1-amino-2-ethenyl-3-(phenylsulfonyl)-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.

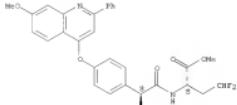
14 ANSWER 2 OF 25 CAPLUS COPYRIGHT 2009 ACS on STN (Continued)
 dimethylhexyl)carbonyl)amino]-2-[(17-methoxy-2-phenyl-4-quinolinyl)oxy]phenylacetyl]amino]-2-ethenyl-, ethyl ester, (12,25)- (CA INDEX NAME)

Absolute stereochemistry.



15 928162-18-7 CAPLUS
 CH₃ Butanoic acid, 2-[(12b)-3,6-dioxo-1-[(1,1-dimethylhexyl)carbonyl]amino]-2-[(4-[(17-methoxy-2-phenyl-4-quinolinyl)oxy]phenyl)acetyl]amino]-4,4-difluoro-, methyl ester, (2S)- (CA INDEX NAME)

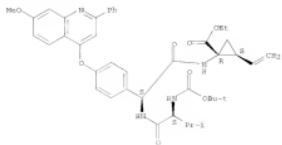
Absolute stereochemistry.



16 928162-18-20-9 CAPLUS
 CH₃ Cyclopropanecarboxylic acid,
 N-[(1,1-dimethylhexyl)carbonyl]-L-valyl-(2S)-2-[(17-methoxy-2-phenyl-4-quinolinyl)oxy]phenylglycyl-1-amino-2-ethenyl-, ethyl ester, (12,25)- (CA INDEX NAME)

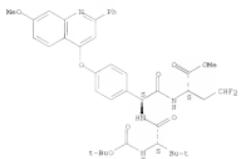
Absolute stereochemistry.

14 ANSWER 2 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



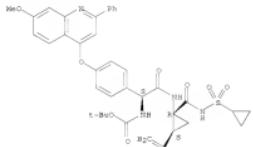
HN 928162-21-4 CAPLUS
 CH Betanazole acid,
 H-[1-(1-dimethylsilyloxy)carbonyl]-3-methyl-L-valyl-(2S)-2-[4-
 [(7-methoxy-2-phenyl-4-quinolinyl)oxy]phenyl]glycyl-2-amino-4,4-difluoro-,
 methyl ester, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



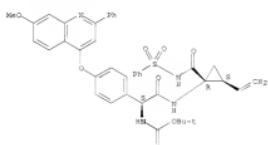
HN 928162-23-0 CAPLUS
 CH Betanazole acid,
 H-[1-(1-dimethylsilyloxy)carbonyl]-3-methyl-L-valyl-(2S)-2-[4-
 [(7-methoxy-2-phenyl-4-quinolinyl)oxy]phenyl]-
 2-oxo-2-[(1S)-1-[(phenylsulfonyl)anilino]butyl]aminoethyl ester, (2S)-
 1,1-dimethylethyl ester (CA INDEX NAME)

14 ANSWER 2 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



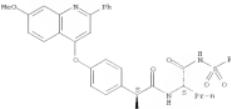
HN 928162-24-1 CAPLUS
 CH Betanazole acid, H-[1-(2S)-2-[(1S,2S)-2-ethoxy-1-
 [(phenylsulfonyl)anilino]carbonyl]cyclopropyl]amino]-1-[4-[(7-methoxy-2-
 phenyl-4-quinolinyl)oxy]phenyl]-2-acetyl-, 1,1-dimethylsilyl ester
 (CA INDEX NAME)

Absolute stereochemistry.



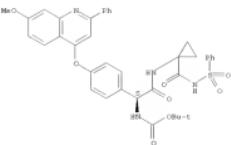
HN 928162-24-2 CAPLUS
 CH Betanazole acid, H-[1-(2S)-2-[(1S)-1-[(cyclopropylacetyl)amino]carbonyl]-
 2-ethoxy-2-[(1S)-1-[(7-methoxy-2-phenyl-4-
 quinolinyl)oxy]phenyl]-2-oxoethyl]-, 1,1-dimethylethyl ester (CA INDEX
 NAME)

Absolute stereochemistry.

14 ANSWER 2 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
 Absolute stereochemistry.

HN 928162-26-9 CAPLUS
 CH Carbamic acid,
 H-[1-(2S)-2-[(1S)-1-[(phenylsulfonyl)anilino]carbonyl]cyclopropyl]-
 2-oxo-2-[(1S)-1-[(phenylsulfonyl)anilino]carbonyl]cyclopropyl]aminoethyl-,
 1,1-dimethylsilyl ester (CA INDEX NAME)

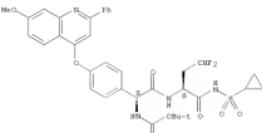
Absolute stereochemistry.



HN 928162-27-0 CAPLUS
 CH Carbamic acid,
 H-[1S]-2-[(1S,2S)-1-[(cyclopropylsulfonyl)amino]carbonyl]-
 2-ethoxy-2-[(1S)-1-[(7-methoxy-2-phenyl-4-
 quinolinyl)oxy]phenyl]-2-acetyl-, 1,1-dimethylsilyl ester (CA INDEX
 NAME)

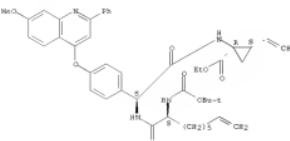
Absolute stereochemistry.

14 ANSWER 2 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



HN 928162-51-0 CAPLUS
 CH Cyclopropanecarboxylic acid, 1-[(2S)-2-[(1S)-2-[(1S,2S)-
 dimethylsilyl]carbonyl]amino]-1-oxo-2-methoxy-1-yl]cyclopropane-2-14-[(7-methoxy-
 2-phenyl-4-quinolinyl)oxy]phenyl]acetyl]amino]-2-acetyl-, ethyl ester,
 (1S,2S)- (CA INDEX NAME)

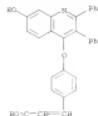
Absolute stereochemistry.



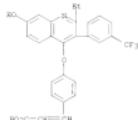
HN 928162-54-2 CAPLUS
 CH 2,5-dimethylcyclohexyl-1,1-bis(2-[(1S)-1-ethoxy-1-carboxylic acid,
 2,5-dimethylcyclohexyl]carbonyl)amino)-4-[(7-methoxy-2-phenyl-4-
 quinolinyl)oxy]phenyl]-2,6-dioxo-, ethyl ester, (1R,4S,7R,12S,15S)- (CA
 INDEX NAME)

Absolute stereochemistry.
 Double bond geometry as shown.

14 ANSWER 4 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

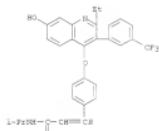


823300-17-6 CAPLUS
CH 2-Propenoic acid, 3-[4-[(2-ethyl-7-hydroxy-3-[(trifluoromethyl)phenyl]-4-quinolinyloxy)phenyl]-4-quinolinyloxy]phenyl- (CA INDEX NAME)

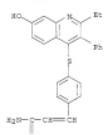


823300-14-7 CAPLUS
CH 2-Propenoic acid, 3-[3-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyloxy)phenyl]-4-quinolinyloxy]phenyl- (CA INDEX NAME)

14 ANSWER 4 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

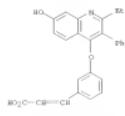


843711-18-6 CAPLUS
CH 2-Propenoate, 1-[(2-ethyl-7-hydroxy-3-[(4-quinolinyloxy)phenyl]phenyl)-3-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyloxy)phenyl]phenyl]- (CA INDEX NAME)

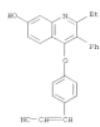


IT 843711-12-7
KLs: RCT (Reagent); RACT (Reagent or reagent)
(preparation of substituted quinoline compds. for use as selective
receptor modulator to treat various diseases)
823300-12-7 CAPLUS
CH Quinoline, 4-[(4-bromophenoxy)-2-ethyl-3-phenyl- (CA INDEX NAME)

14 ANSWER 4 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

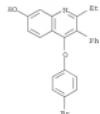


823711-16-4 CAPLUS
CH 2-Propenoate, 1-[(2-ethyl-7-hydroxy-3-[(trifluoromethyl)phenyl]-4-quinolinyloxy)phenyl]-3-[(2-ethyl-7-hydroxy-3-[(trifluoromethyl)phenyl]-4-quinolinyloxy)phenyl]- (CA INDEX NAME)



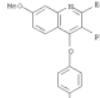
823711-17-5 CAPLUS
CH 2-Propenoate, 1-[(2-ethyl-7-hydroxy-3-[(trifluoromethyl)phenyl]-4-quinolinyloxy)phenyl]-3-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyloxy)phenyl]- (CA INDEX NAME)

14 ANSWER 4 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



823711-18-17 CAPLUS
KLs: RCT (Reagent); RACT (Reagent); RPP (Synthetic preparation); RPP (Preparation); RACT (Reagent or reagent)
(preparation of substituted quinoline compds. for use as selective
receptor modulator to treat various diseases)

823300-22-7 CAPLUS
CH Quinoline, 4-[(4-bromophenoxy)-2-ethyl-7-methoxy-3-phenyl- (CA INDEX NAME)



823300-22-7 CAPLUS
CH 2-Propenoic acid, 3-[(2-ethyl-7-methoxy-3-phenyl-4-quinolinyloxy)phenyl]-, ethyl ester (CA INDEX NAME)

14 ANSWER 7 OF 25 CAPTURE COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 82011570357 CAPLUS

DOCUMENT NUMBER: 142121098

TITLE: Ligands Using Peptide Interaction Profiling

AUTHOR(S): Bockstra, William J.; Patel, Rati S.; Liang, Xi; Borchardt, Robert T.; Kao, Ming-Jui; Liao, Yen-Jui; Wilson, Timothy M.; Jansson, Marie A.; Kadwell, Sue H.; Miller, Lisa A.; Pearson, Kenneth R.; Surman, J.; Chiu, Yen-Chang; Chang, Chia-Chang

CORPORATE SOURCE: GlaxoSmithKline Research Development, Research Triangle Park, NC, 27705-3739, USA

SOURCE: Journal of Medicinal Chemistry, Vol. 49, No. 12, 2006, pp. 3245-3247

JOURNAL: Journal of Medicinal Chemistry

DOCUMENT TYPE: Article

LANGUAGE: English

ORIGINAL SOURCE(S): CA/SEARCH 142121098

AB Traditional approaches to discovery of selective estrogen receptor modulators (ERMs) have relied on cell-based screening and cell-based estrogen response element-driven assays to identify compounds that are estrogenic but nonselective. In breast and uterine tissues, 70 estrogenic compounds (ERMs) were identified using a cell-free microsphere-based binding assay to rapidly characterize ERMs in interactions with conformation-sensing cofactor or phage display peptide.

Peptide profiles of contraindicated triflazene were compared to known estrogen receptor ligands to develop a method to discover potent quinoline-based ligands with minimal side effects on cell stimulation.

IT 820300-07-9 820300-08-09 820300-09-07 820300-10-0 820300-11-1 820300-12-2 820300-13-4 820300-14-19 820300-15-02 820300-16-3 820300-17-4 820300-18-5 820300-19-6 820300-20-7 820300-21-8 CAPLUS

EE PAC (Pharmaceutical activity); 200 (Synthetic preparation); 200 (Pharmacological activity); 2002 (Preparation); UGC (Uses)

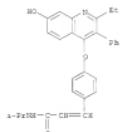
KJ 820300-07-8 CAPLUS

CH 2-Propenoic acid, 3-[4-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyloxy)oxy]phenyl]- (CA INDEX NAME)

CH 820300-07-8 CAPLUS

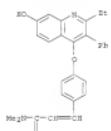
CH 2-Propenoic acid, 3-[4-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyloxy)oxy]phenyl]- (CA INDEX NAME)

14 ANSWER 7 OF 25 CAPTURE COPYRIGHT 2008 ACS on STN (Continued)



KH 820300-10-3 CAPLUS

CH 2-Propenoic acid, 3-[4-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyloxy)oxy]phenyl]- (CA INDEX NAME)

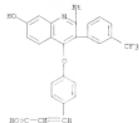


KH 820300-11-4 CAPLUS

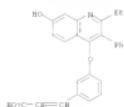
CH 2-Propenoic acid, 3-[4-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyloxy)oxy]phenyl]-1-oxo-2-(phenyl)- (PCL) (CA INDEX NAME)

14 NUMBER 7 OF 23 CAPTION COPYRIGHT 2008 AGS OR STH (Continued)

(Cont'd next)



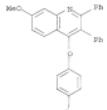
720 020300-14-7 CAPLOS
C2 2-Propenoic acid, 3-[3-[(2-ethyl-7-hydroxy-3-phenyl-4-
quinoxalinyl)oxy]phenyl]- (CA INDEX NAME)



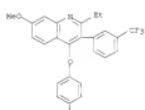
PN 828300-15-9 CAPLUS
 CS 7-Quinolinol, 4-[4-(2-(dimethylamino)ethoxy)phenoxy]-2-ethyl-3-phenyl-1-
 CA INDEX NAME

14 ANSWER 7 OF 25 CAPTION COPYRIGHT 2009 ACS on 979 (Continued)

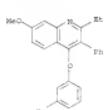
(Cont'd next)



922 828300-20-5 CAPLUS
C9 Quinoline, 4-(4-bromophenoxy)-2-ethyl-7-methoxy-3-(3-(trifluoromethyl)phenyl)- [CA INDEX NAME]

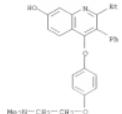


NN 828300-21-6 CAPTURS
CN Quinoline, 4-(3'-bromophenoxy)-2-ethyl-7-methoxy-3-phenyl- (CA INDEX)



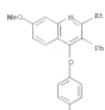
RR 828300-22-7 CAPLUS
C9 2-propenoic acid, 3-[4-[(2-ethyl-7-methoxy-3-phenyl-4-quinolinyl)oxy]phenyl]-, ethyl ester (CA INDEX NAME)

(Continued)



17 828300-18-1P 828300-19-2P 828300-20-5P
828300-21-6P 828300-22-7P 828300-23-8P
828300-24-9P 828300-25-0P

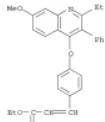
El: ECT (Ectant); SM: (Synthetic preparation); PREP: (Preparation); E&C: (Echant or reagent);
 (discovery of novel quinoline-based estrogen receptor ligands using peptide interaction profiling)
 8528300-15-1 CARLOS
 QUINOLINE, 4-(4-bromobenzoyl)-2-ethyl-7-methoxy-3-phenyl- (CA INDEX



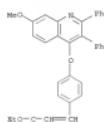
RR 828300-19-2 CAPIUS
CN Quinoline, 4-(4-iodophenoxy)-7-methoxy-2,3-diphenyl- (CA INDEX NAME)

14 ANSWER 7 OF 25 CAPTION COPYRIGHT 2008 ACR on STN (Continued)

(Cont'd next)

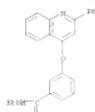


HN 828300-23-8 CAPLUS
CN 2-Propenoic acid,
3-[4-[(1-methoxy-2,3-diphenyl-4-quinoxinyl)oxy]phenyl]-
ethyl ester (CA INDEX NAME)



RR 028300-24-9 CAPLUS
CN 2-Propenoic acid,
3-[4-[2-ethyl-7-methoxy-7-(7-trifluoromethyl)phenyl]-4-
quinalinyl]oxyphenyl]-, ethyl ester (CA INDEX NAME)

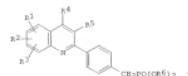
14 ANEMLR 14 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
as benzodiazepine receptor ligands)
15 178300-57-3 CAPLUS
16 178300-57-3 CAPLUS
17 178300-57-3 CAPLUS



L4 ANIMER 15 OF 25 CARLOS COFRAGNET 2000 ACS ON STN
ADDRESS NUMBER: 1991493504 CARLOS
DOCUMENT NUMBER: 11234567890
TITLE: Preparation of quinolines as peptidomimetics and
antidiabetics
INVENTOR(S): Mysa, Katsuhiko; Shioi, Yasuo; Tsubada, Toshihiko
Kondo, Toshiaki; Yamada, Kuniyuki; Fujii, Izumi; Yamada,
Osaka Pharm Co Ltd, Japan
PATENT ASSIGNEE(S): Jpn. Kokai Tokkyo Koho, 13 pp.
SOURCE: JP-A-131035
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
PUBLICATION NUMBER: 1991-04-11
PATENT INFORMATION:

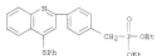
PATENT NO.	KIND	DATE	APPLICATION NO	DATE
JP 05043589	A	19930223	JP 1992-13106	19920120
PRIORITY APPLN. INFO.:			JP 1991-102184	A1 19910205

OTHER SOURCE IS: **MAPAT 319, 9536**



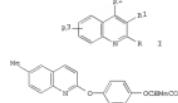
17 149133-10-2P
 Rb: BPH (Synthetic preparation); PREP (Preparation)
 (preparation of, as hypoglycemic and antidiabetic agent)
 RN 149133-10-2
 CN Phos(phenic acid, [1-[4-[(phenylthio)-2-quinolinyl]phenyl]ne-
 diethyl
 ester (ICL) (CA INDEX NAME)

14 ANSWER 15 OF 25 CAP1035 COPYRIGHT 2008 AOS on 8798 (Continued)

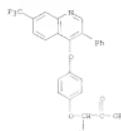


14 ANSWER 16 OF 25 CAPTION COPYRIGHT 2008 ACS on 979

PATENT INFORMATION
PATENT NO. KIND DATE APPLICATION NO. DATE
DE 3101544 A1 19920819 DE 1991-3101544 19910120
PRIORITY APPLN. INPO. : DE 1991-3101544 19910120
OTHER SOURCE(S): CASREACT 97:198123



14 ANSWER 16 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

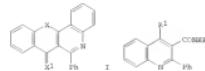


220 6559-73-8 CAPLUS
Propionic acid, 2-[(4-((2-phenyl-4-quinolyl)oxy)phenyl)-, ethyl ester
(CA INDEX NAME)



14 ANSWER 17 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESION NUMBER: 1978122704 CAPLUS
DOCUMENT NUMBER: 88122704
ORIGINAL REFERENCE NO.: 87426454, 26464
TITLE: Hetero- and structure of some new heterocyclic
analogues of benzothiophene
AUTHOR(S): Inst. Chem., Jagiellonian Univ., Krakow, Pol.
SOURCES: University Nankai, Universitetu Jagiellonskiego, Krakow, Poland
DOCUMENT TYPE: English
LANGUAGE: English
COUNTRY: POLAND ISSN: 0373-0146
CODE: 124041 ISSN: 0373-0146

DOCUMENT TYPE: English
LANGUAGE: English



AB Condensed quinolines I ($X = O, S, X1 = Cl$) were obtained by treating II ($R = Ph, R1 = Cl$) with Ph3SiCl and cyclizing II ($R = Ph, R1 = Cl$) with phosphorus pentaphosphoric acid. Treatment of II ($R = Ph, R1 = XPh$) with Ph3SiH and cyclization of II ($R = Ph, R1 = XPh$) gave I ($X = O, S, X1 = NH$), which were converted to II ($X = O, S, X1 = NH$) with Ph3SiH and Ph3SiCl.
17 65031-26-7 65032-26-9 65031-30-3P
Eliel RCG (Reactant); BPR (Synthetic preparation); P3SP (Preparation); PACT (Reactant or reagent)
Eliel RCG (Reactant); BPR (Synthetic preparation of)
KH 65031-26-7 CAPLUS
3-Quinolincarboxamide, 4-phenoxyl-2-phenyl- (CA INDEX NAME)



18 65031-28-3 CAPLUS
3-Quinolincarboxamide, 4-phenoxyl-2-phenyl- (CA INDEX NAME)

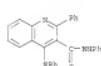
14 ANSWER 17 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



220 65031-30-3 CAPLUS
3-Quinolincarboxamide, 2-phenyl-4-(phenylthio)- (CA INDEX NAME)

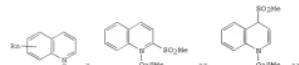


220 65031-32-4 CAPLUS
1-Quinolincarboxamide, N,2-diphenyl-4-(phenylthio)- (CA INDEX NAME)



14 ANSWER 18 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESION NUMBER: 1977156784 CAPLUS
DOCUMENT NUMBER: 87426515a, 26522a
ORIGINAL REFERENCE NO.: 87426515a, 26522a
TITLE: The reaction of heterocyclic N-oxide with acid
chlorides. Part 1. The reaction of quinoline
N-oxide with sulfonyl acid chloride and potassium
cyanide
AUTHOR(S): Shinkai, Shinsada, Moraki
SOURCES: Shinkai Coll. Pharm., Shinsada, Japan
Yakuza, T., Tsuru, T., Shinkai, S., Moraki, S., 627-640
Jpn. J. Pharm. (TOKUSAI); ISSN: 0931-614X
DOCUMENT TYPE: Journal
LANGUAGE: Japanese



AB Reaction of 17 quinoline oxides I (e.g., $R = H, Me, NO_2, Ph, Cl$) with $ClSO_2Me$ and KCN gave the 2-(methylsulfonyl)quinolines or, when the α -position was substituted, the 4-(methylsulfonyl) derivative via elimination of HO_2SMe from the intermediates II or III.

17 64495-42-1 CAPLUS
Eliel RCG (Preparation)
KH 64495-42-1 CAPLUS
Quinoline, 2-phenyl-4-(phenylsulfonyl)- (CA INDEX NAME)



18 64495-43-2 CAPLUS
Quinoline, 2-(4-methylphenyl)-4-(phenylsulfonyl)- (CA INDEX NAME)

14 ANHED 22 OF 25 CAPSULE. COPYRIGHT 2000 ACS ON STN
 ACCESSION NUMBER: 1998-25579 CAPSULE
 ORIGINAL PUBLICATION: 1998-25579
 ORIGINAL REFERENCE NO.: 5244657-0-1
 SYNTHESIS OF KINETIC ANALOGS. I
 Yano, T.; Shioya, Masayuki; Mito, Mototsugu;
 Tochizaki, Takahashi, Tadashi; Murakami, Shunji
 Department of Chemistry, Faculty of Science, Japan
 Corporate Source: Bulletin of the Chemical Society of Japan (1357), 30,
 1941-1942
 DOI: 10.1246/bcsj.1357.2617
 SOURCE: BUNKA, ISSN: 0009-2617
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 ABSTRACT: It is reported that 2,4-disubstituted 3-methylpyridazines (II) are
 prepared by condensing 4-methylpyridine and
 α -chloro- β , β -dihydronaphthalene-1,4-dione (I)
 resp., with various amines. Pyridine I prepared by this method were
 α -substituted, recrystallized temperature and time (hr.), λ , yield, n.p.

IT 102241-29-2 |Derived from data in the 6th Collective Formula Index (1957-1961)|
320 1Q2241-29-2 CAPLOS



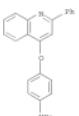
88 612872-11-7 CAP/PS



14 ANSWER 24 OF 25 CARLSB COPYRIGHT 2008 ACS on STN (Continued)
 mol. Pd(OAc)₂ gives 53% V, 0.07 mol. I and 0.04 mol. Pd(OAc)₂ gives 55 V, 228 IV,
 and 1.7 g. [Pd(OAc)₂]. The Pd(OAc)₂/Pd(OAc)₂ ratio is 3.8 g. I and 1.7 g.
 17 840719-92-2 CAPLUS Quinoline, 6-chloro-4-phenoxy-3-phenyl-
 HL PREP (Preparation)
 840719-92-2 CAPLUS
 Quinoline, 6-chloro-4-phenoxy-3-phenyl- (CA INDEX NAME)



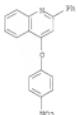
14 ANSWER 25 OF 25 CARLSB COPYRIGHT 2008 ACS on STN (Continued)
 ACQUISITION NUMBER: 1928120282 CARLSB
 DOCUMENT NUMBER: 22120202
 DOCUMENT REFERENCE NO.: 122020224
 TITLE: Quinoline derivatives. VIII. Compounds of
 2-phenyl-4-hydroxyquinoline
 AUTHOR(S): K. H. Borchardt, R. K. Koenig
 SOURCE: Journal für Praktische Chemie (Leipzig) (1928), 119,
 42-5
 DOCUMENT TYPE: Journal
 LANGUAGE: German
 REFERENCE: C. A. 22, 426.
 An 855087-34-2P, Quinoline, 4-(p-anisophenoxy)-2-phenyl- derivative, m. 90°²,
 various salts of this and the following are described. 4-Phenyl-
 derivatives, yellow, m. 252°,
 4-n-Cresoxy derivative, m. 241°,
 4-(p-methoxyphenyl) derivative, m. 240°,
 4-(p-ethoxyphenyl) derivative, m. 241°,
 4-(p-nitrophenyl) derivative, m. 242°, All but the last two
 derivatives are described in 855087-34-2P, Quinoline, 4-(p-anisophenoxy)-2-phenyl-
 854095-26-1 CAPLUS Quinoline, 4-(p-anisophenoxy)-2-phenyl-
 Quinoline, 4-(2-isopropyl-5-methoxybenzyl)-2-phenyl- 854096-70-7P
 Quinoline, 4-(2-isopropyl-5-methoxybenzyl)-2-phenyl- 854096-92-9P
 HL PREP (Preparation)
 855087-34-2 CAPLUS
 Quinoline, 4-(p-anisophenoxy)-2-phenyl- (3C1) (CA INDEX NAME)



3H 854085-26-1 CAPLUS
 Quinoline, 2-phenyl-4-m-toloxyl- (3C1) (CA INDEX NAME)

14 ANSWER 25 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

22 854085-26-1 CAPLUS
 Quinoline, 4-(p-anisophenoxy)-2-phenyl- (3C1) (CA INDEX NAME)



22 854094-43-9 CAPLUS
 Quinoline, 4-(2-isopropyl-3-methylphenoxy)-2-phenyl- (3C1) (CA INDEX NAME)



22 854094-70-3 CAPLUS
 Quinoline, 4-phenoxy-2-phenyl- (CA INDEX NAME)

14 ANSWER 25 OF 25 CARLSB COPYRIGHT 2008 ACS on STN (Continued)

2H 854094-92-9 CAPLUS
 Quinoline, 4-(o-methoxybenzyl)-2-phenyl- (3C1) (CA INDEX NAME)



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